QLib - A Matlab Package for Quantum Information Theory Calculations with Applications

S. Machnes
School of Physics and Astronomy, Beverly and Raymond Sackler Faculty of Exact Sciences, Tel-Aviv University, Tel-Aviv 69978, Israel
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Developing intuition about quantum information theory problems is difficult, as is verifying or ruling-out of hypothesis. We present a Matlab package intended to provide the QIT community with a new and powerful tool-set for quantum information theory calculations. The package covers most of the "QI textbook" and includes novel parametrization of quantum objects and a robust optimization mechanism. New ways of re-examining well-known results is demonstrated. QLib is designed to be further developed and enhanced by the community and is available for download at `www.qlib.info`

I. MOTIVATION

Advances in theory are often fore-shadowed by intuition. But the mathematical structures governing multipartite and even bipartite states and unitary transformations are complex, which makes many problems difficult to explore and intuition hard to develop. Analyzing problems analytically is often a time-consuming process. Validation of hypothesis is laborious and searching for counter-examples is a lengthy endeavor. The QIT community will probably benefit from tools to accelerate these processes.

The use of computers for theoretical mathematics is a well established, with a specialized journal [2], textbooks [3, 4, 5] and numerous papers. Wolfram research defines *experimental mathematics* as "a type of mathematical investigation in which computation is used to investigate mathematical structures and identify their fundamental properties and patterns" [6]. Bailey and Borwein[7] use the term to mean the methodology of doing mathematics that includes the use of computation for

- Gaining insight and intuition
- Discovering new patterns and relationships
- Using graphical displays to suggest underlying mathematical principles
- Testing and especially falsifying conjectures
- Exploring a possible result to see if it is worth formal proof
- Suggesting approaches for a formal proof
- Replacing lengthy hand derivations with computer-based derivations
- Confirming analytically derived results

As the benefits of tools such as Mathematica, Matlab and Maple are clear, there is strong indication that field-specific software for experimental theoretical quantum information would be advantageous. QLib [1] is an attempt to provide such a tool.

II. OVERVIEW OF CAPABILITIES

QLib provides the tools to manipulate density matrices, separable states, pure states, classical probability distributions (CPDs) as well as unitary and Hermitian matrices. All of which are supported with any number of particles, and any number of degrees of freedom per particle. The following functions are provided to manipulate these objects:

- **Entanglement calculations**: pure state entanglement, concurrence, negativity, tangle, logarithmic negativity, entanglement of formation, relative entanglement, robustness, PT-test (Peres Horodecki), Schmidt decomposition and singlet fraction.
- **Entropy**: Shannon, Von Neumann, linear entropy, relative entropy, participation ratio, purity
- **Measurements**: Orthogonal (to multiple collapsed states or to a single mixture) , POVM, weak measurements
- **Object transformation:**
  - Reorder particles, partial trace, partial transpose
  - Transform objects to/from the regular representation to a tensoric representation with one index per particle if the original object was a vector, or two indexes per particle if the object was a matrix
  - Convert to/from computational base to the base of SU(n) generators
- **Distance measures**: Hilbert-Schmidt, trace distance, fidelity, Kullback-Leibler, Bures distance, Bures Angle, Fubini-Study
- **Miscellaneous**: Majorization, mutual information, spins in 3D, famous states, famous gates

QLib provides **parametrizations for all objects of interest**, density matrices, separable states, pure states, CPDs, Hermitian matrices and unitary matrices. In other words, these object are representable as points in a parameter space. This allows, for example, to generate random separable states or random unitary matrices. For details of each parametrization and its theoretical background, please refer to the on-line help. As an example, details of two unitary-matrix parametrizations and of one separable density matrix parametrization are presented in IV. The **robust optimization capabilities** provided with QLib, allows searching for extrema of functions defined over these spaces. The optimization is performed by alternating stages of hill-climbing and simulated annealing while applying consistency requirements to the output of the stages. Current experience with the optimization feature suggests that the search succeeds in locating the global extrema in a surprising majority of the cases [17].

Finally QLib provides a wide selection of general purpose utilities which, while are not quantum-information specific, go a long way towards making the use of QLib productive and simple:

- Linear algebra: Gram Schmidt, spanning a matrix using base matrices, checking for linear independence, etc.
- Numerics: Approximately compare, heuristically clean-up computation results from tiny non-integer and/or tiny real/imaginary parts, etc.
- Graphics: Quickly plot out functions in 2 and 3d, smoothing and interpolation techniques for noisy or sparse data, etc.

III. GETTING STARTED

QLib, available at `www.qlib.info`, has been designed for easy use. An *Installation Guide* and a *Getting Started Guide* are available on the website, and over a dozen demos are provided as part of QLib, to help you get started.

In addition, on-line help is available: simply type `help qlib` at the Matlab prompt for an overview of functionality or get function-specific help, e.g. `help partial_trace`.

Finally, user forums are available to ask questions and discuss QLib issues, and forms are provided to request new features or report bugs.

IV. SAMPLE APPLICATIONS

Following are a number of QLib usage example which were selected both for their ability to demonstrate QLib capabilities and for their relatively simple structure and simple theoretical background, so that they may be quickly understood by a wide range of readers.

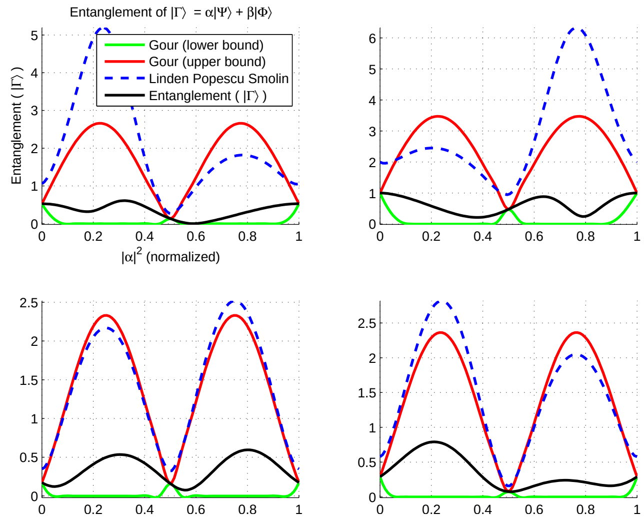

Figure 1: (color on-line) Limits on entanglement of superpositions of randomly selected states. Gour appears to match the goal function for at both ends and when $|\alpha| = |\beta|$. Generally speaking, Gour is indeed tighter than LPS, but not always (note the top-left sub-figure at $|\alpha|^2 = 0.55$). Also of note is the complex behavior exhibited by the entanglement of superposition and the relative un-tightness of existing bounds.

A. Entanglement of Superpositions

Recently, some work has been done regarding the entanglement of superpositions

$$|\Gamma\rangle = \alpha|\Psi\rangle + \beta|\Phi\rangle \quad (1)$$

An upper limit to the entanglement of $|\Gamma\rangle$ has been proposed by Linden, Popescu and Smolin [8]. Further work by Gour [9] added a tighter upper bound and a lower bound. Unfortunately, the analytical form of these bounds make it difficult to get a good intuitive feel as to whether they are relatively tight or whether there is still significant room for improvement. QLib provides us with convenient tools with which to explore the problem. See figure 1.

To create the graphs above, QLib's basic primitives have been used (computation of entanglement for a pure state, normalization of a pure state, etc), as was the capability to generate random pure states. Finally the optimization capabilities are also put to use, as Gour's bounds are defined in terms of maximizing a function over a single degree of freedom for given Ψ,Φ, α and β, which requires that every point along the Gour limit lines above be computed by an optimization process.

B. Maximally Entangled Mixed States

Over the years there has been keen interest in the question of MEMS, Maximally Entangled Mixed States, which cannot be made more entangled (as measured by

some measure) with any global unitary transformation [13, 14, 15]. QLib can assist in exploration of this problem by searching for the most-entangling unitary transformation. Parametrization of unitary transformations is done either by generalized Euler angles [16] or with the more naive

$$U = e^{i \sum_{k=1}^{n^2} \theta_i \mathbf{g}_i} \tag{2}$$

with $\mathbf{g}_i$ being the $U(n)$ generators.

In this particular example, we have explored the maximal entanglement possible for the separable diagonal density matrix

$$\begin{pmatrix} p & 0 \\ 0 & 1-p \end{pmatrix} \otimes \begin{pmatrix} q & 0 \\ 0 & 1-q \end{pmatrix} \tag{3}$$

QLib can help discover the dependency of the maximal entanglement on p, q by locating the MEMS associated with the initial density matrix and visualizing various options for p, q dependence. See figure 2.

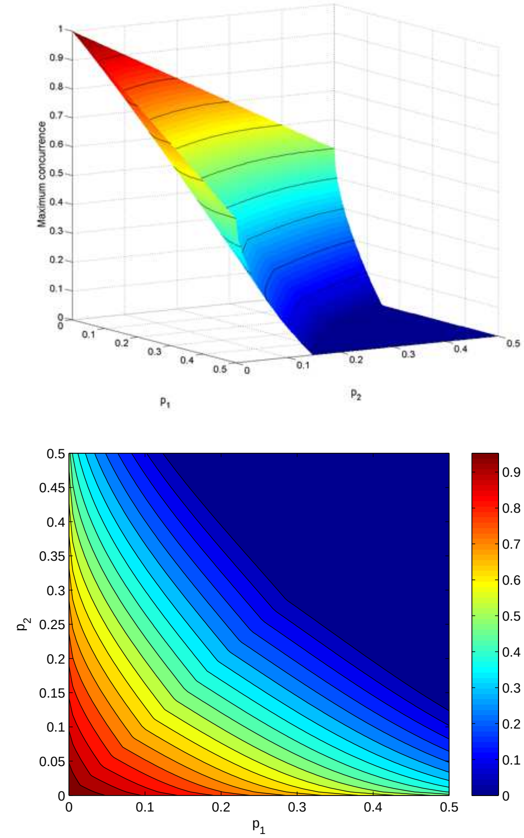

Figure 2: (color on-line) Maximal concurrence for eq. 3. The $(p, q) = [0..0.5, 0..0.5]$ space was explored with a resolution of 0.005, for a total of 10,000 points, for each of which an optimization of the concurrence over the space of SU(4) unitaries has been performed. The maximal concurrence is shown both as a function of p and q (in 3d, above), and as a contour plot (below) showing the dependence of the maximal concurrence on the trace distance between the single-particle initial density matrix, $\begin{pmatrix} p & 0 \\ 0 & 1-p \end{pmatrix}$, and the fully mixed state for a single qubit $\begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$.

C. Bloch "Hyper-sphere"

It is well known that a single qubit may be represented using the $U(2)$ generators as

$$\rho_{1\,qubit}(\overrightarrow{n}) = \frac{1}{2}\left(\mathbf{1} + \overrightarrow{n} \cdot \overrightarrow{\sigma}\right) \tag{4}$$

with a pure state iff $\|\overrightarrow{n}\| = 1$. This suggests a trivial generalization to higher dimensions as follows

$$\rho(\overrightarrow{n}) = \frac{1}{2}\mathbf{1} + \sum_{\mathbf{i=1}}^{\mathbf{n^2-1}} c_i \mathbf{g}_i \tag{5}$$

with $\mathbf{g}_i$ being the $SU(n)$ generators, with the assumption that if $\sum_{\mathbf{i=1}}^{\mathbf{n^2-1}} |c_i|^2 = \frac{1}{4}$ then the density matrix represents a pure state.

Utilizing QLib's parametrization capabilities, we shall generate a large number of random pure states, separable states and general density matrices and plot the $2d$ projections of the resulting Bloch "hyper-sphere", i.e. scatter plots of two components of $\overrightarrow{c}$. It is evident from figure 3 that no such trivial generalization is possible, and that the geometry of the problem is far more complex that can be naively guessed.

D. Additivity of entanglement and entropy measures

Another simple use of QLib is to experimentally test the additivity of entropy and entanglement measures

$$E(\rho_1 \otimes \rho_2) \stackrel{?}{=} E(\rho_1) + E(\rho_2) \tag{6}$$

By randomly generating multiple ρ_1-s and ρ_2-s and checking the additivity attribute for each, we can form a reliable hypothesis regarding the behavior of the measure in question. Moreover, by extremizing $E(\rho_1 \otimes \rho_2) - E(\rho_1) - E(\rho_2)$ over all possible ρ_1,ρ_2 one may reach an even more well-founded conclusion. Of particular interest is the relative entanglement measure [10]

$$E_R = \inf_{\sigma \in SEP} tr\, \rho \left(\log\rho - \log\sigma\right) \tag{7}$$

which is a generalization of the classical relative entropy

$$S(p|q) = tr\, p(\log p - \log q) \tag{8}$$

It is known that E_R is non-additive [11].

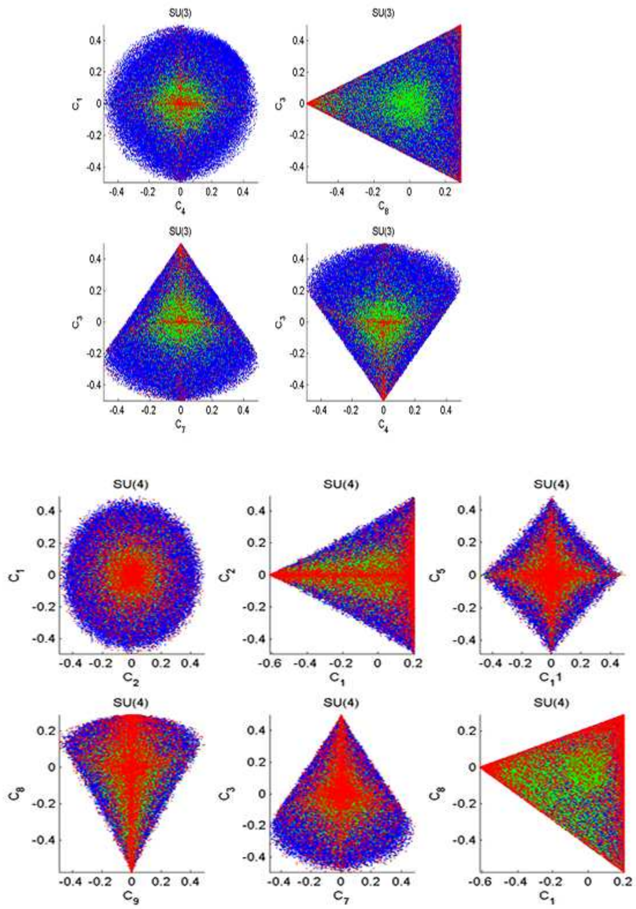

Figure 3: (color on-line) $2d$ projections of the SU(3) and SU(4) Bloch "hyper-spheres". Blue dots indicate general density matrices. Green are separable states and red dots indicate pure states.

To compute E_R, one must be able to compute $\inf_{\sigma \in SEP}$, which in turn requires parametrization of the separable space. In QLib this is achieved using the observation of P. Horodecki [12], that the separable space is convex, and thus each point within is constructable as a linear interpolation of a finite number of extremal points of that space, as per the Caratheodory theorem. Therefore, to parametrize all separable density matrices of dimension d, one may parametrize d^2 separable pure states of the same dimensionality $|\phi_i\rangle$ and a classic probability distribution $\{p_i\}$ to specify the mixing, resulting in the parametrization

$$\rho = \sum_{i=1}^{d^2} p_i |\phi_i\rangle\langle\phi_i|. \tag{9}$$

The numerical study of E_R additivity clearly indicate that the relative entanglement is super-additive, i.e.

$$\text{hypothesis:} \quad E_R(\rho_1 \otimes \rho_2) > E_R(\rho_1) + E_R(\rho_2) \tag{10}$$

V. LOOKING FORWARD - A COMMUNITY EFFORT

QLib is distributed as free software. The word "free" does not only refer to price; primarily it refers to freedom: You may run the program, for any purpose, study how it works, adapt it to your needs, redistribute copies and improve the program.

It is our hope is that QLib will evolve into a group effort, maintained, nurtured and grown by the Quantum Information community, for the benefit of us all. For that purpose, we have licensed QLib under the GPL, or GNU Public License, which sets-up both the freedom to use the software, and the requirement that any enhancements made to QLib be released back to the community. Code which uses QLib, but is not part of it, may, of course, remain private. For more information regarding these issues, see the licensing section of the QLib website.

Several tools are available on the website to facilitate joint development of future versions: Forums, a bug tracking system, a feature request form and a mailing list.

The direction future QLib development will take shall be determined by you, its users.

Acknowledgments

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